



Elite Study Program in Macromolecular Science

Start Module M033

**Modern Research Topics in
Macromolecular Science**

Faculty of the Elite Study Program

Winter term 2013/14

The scope of the Start Module “Modern Research Topics in Macromolecular Science” is to introduce the students, coming from different backgrounds, to various facets of the broad and interdisciplinary field of Macromolecular Science. It is intended that the students will get a basic understanding of underlying concepts, technical terminology and methodologies in the individual subfields of Macromolecular Science beside their main focus. The offered topics cover the fields macromolecular chemistry, colloidal chemistry, biopolymers, biochemistry, polymer physics, biophysics, polymer technology, polymer engineering, and theory and simulation of macromolecules. The students individually select 8 topics (4 of topic block A and 4 of topic block B) from ca. 15 offered topics. Each separate topic has a length of ca. 10 hours and includes lectures, seminars and laboratory tours. In addition the students will have a tour and brief introduction of the research facilities.

A: Complex functional nanofiber nonwovens for advanced applications

Andreas Greiner, Macromolecular Chemistry II

Polymer nanofiber nonwovens have numerous applications in filtration, textiles, medicine, pharmacy, agriculture, catalysis, and composites. The performance of nanofibers nonwovens can be engineered by process parameters and by the chemistry of the polymers, which will be the topic of the lectures. Particular focus will be on formulations for electrospinning, post-spinning modifications of nanofibers, structural analysis, and application-related property analysis.

Time frame: 3.4.2014 or alternatively 8.4.2014 (1 full day)

A: Color Formation in Organic Light Emitting Devices (OLEDs) - A Combined Chemistry and Physics Approach

Peter Stroehriegl, Macromolecular Chemistry I

Anna Köhler, Experimental Physics II

Colors have attracted people for thousands of years. In the first part of the interdisciplinary course, a short introduction in the basics of color formation and color mixing will be given. Afterwards, the principles of Organic-Light Emitting Devices (OLEDs) will be introduced with special emphasis on the different materials used.

The second part of the course gives an introduction to the photophysics of OLEDs. In such devices the physical principles of energy transfer from a host material to a guest molecule are used to generate different colors in an energy efficient way. The detailed understanding of the photophysics of organic semiconductors has paved the way to the commercialization of full color OLED-displays.

Time frame: 20.03., 21.03., or 24.03. (1 full day)

A: Biorelevant Functional Polymers

Seema Agarwal, Macromolecular Chemistry II

Biorelevant polymers are speciality polymers of either natural or synthetic origin, which find applications in medicine, pharmacy, food, agriculture, and packaging. Some of the important polymers of this class are: biodegradable polymers, antibacterial polymers, polymers for gene transfection, and tissue engineering. This module will provide a basic overview of biorelevant polymers including biobased and petrobased materials: why and where we require these polymers including examples also from the everyday life. The module will be highlighted with an example from our laboratory to show how a lab curiosity can become a product.

Lab course: The module includes a 3 hrs lab course regarding special characterization methods used for biorelevant polymers.

Time frame: 07.04. or 08.04. (1 full day)

A: Design of supramolecular architectures for functional materials

Hans-Werner Schmidt, Andreas Bernet, Macromolecular Chemistry I, Bayreuther Institut für Makromolekülforschung (BIMF)

A major challenge in polymer science, with respect to novel functional and even multifunctional materials, is the understanding and control of hierarchical structured supramolecular polymers and nano-objects created by (macro)molecular self-assembly. Such complex self-assembled structures will provide constant progress in materials science and play a key role for innovative solutions. Our goal is to fine-tune specific and complex functionality across all length scales (nano to macro) through molecular design and novel hierarchically structured systems. In this context, we explored in the past years the design and structure-property relations of molecules capable to self-assemble into supramolecular nano-fibers and nano-objects. The molecules were for example tailored to function as nucleating/clarifying agents for semi-crystalline polymers, as charge storage additives in electret materials, as nano-fibers for filtration applications and as efficient organo- and hydrogelators.

Time frame: according to students' suggestions (1 full day)

A: Microfluidics

Stephan Förster, Physical Chemistry I

Microfluidics has developed in an established technology for handling very small liquid volumes down to nanoliters. The main drivers are the *lab-on-a-chip* technology to analyze very small quantities of biological samples, and *microreactors* for performing continuous chemical reactions.

In this module we will give an introduction into the basics of microfluidics, build microfluidic chips by soft-lithography or 3D-printing, and perform experiments such as ultrafast mixing experiments, the production of polymer microfibers, or the generation of water jets of just a few micrometer diameters.

Time frame: to be announced (1 full day)

A: Interactions and Nano-Mechanics in Polymer Systems

Andreas Fery, Georg Papastavrou, Physical Chemistry II

Interfacial forces determine many properties like friction, adhesion, or wetting. In recent years, the atomic force microscope (AFM) has developed into a versatile tool for measuring such forces at the nanometer scale with force resolutions in the order of few tenths of a pico-Newton. Such force measurements allow not only to determine the interaction on the level of single polymer chains but as well to explore mechanical properties of nano- and colloidal objects not accessible by other techniques.

In this module we will demonstrate different experimental approaches based on the AFM. The basic principles governing the stretching response of linear polymers, starting from the Gaussian chain model, will be covered as well as the desorption processes of adsorbed polymers from a solid substrate, which allows to probe the interactions on the monomer level. Models describing the mechanic response of polymer capsules or other nano- to micrometer sized structures under external forces represent another important topic.

Upon interest of the participants it will be possible to arrange a practical demonstration of single molecule and other force experiments with the AFM at the end of the module.

Time frame: to be announced (1 full day)

A: Multifunctional Colloids - From Simple Building Blocks to Modern Devices

Matthias Karg, Markus Retsch, Physical Chemistry Department

Colloidal particles represent a materials class with a vast range of composition, size, and shape. The unique properties of colloids can mainly be related to their enormous surface to volume ratio and differ significantly from their respective bulk materials. The functionality of such particles can be further enhanced by self-assembly of such building blocks into regular films or arrays, which for instance are known as colloidal crystals.

In this module we give a detailed introduction into the synthesis, characterization and application of colloidal particles. We will focus on a range of materials such as polymers, metals, and metal oxides, which can also be combined to yield composite materials. Important concepts in colloidal science, in particular the stability of colloidal dispersions and forces influencing colloidal stability, will be introduced. The relevance of these concepts will be discussed in the light of self-assembled materials consisting of colloidal building blocks. Such materials are promising platforms for modern sensors and photovoltaic devices.

Time frame: 24.3., 25.3., or 27.3. (1 full day)

B: Principles of Selforganization

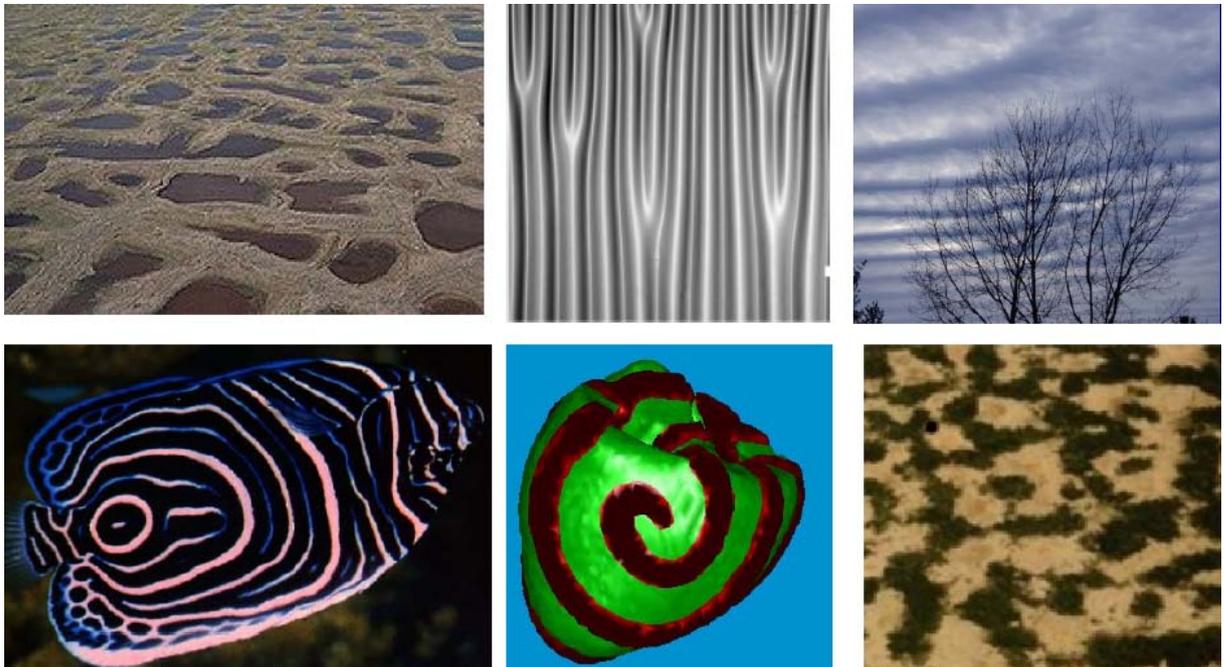
Walter Zimmermann, *Theoretical Physics I*

Patterns are ubiquitous in nature. Stripe patterns, for instance, are found in biology (skin pattern ...), chemistry (Turing), Physics (convection, Taylor-vortices, wrinkles ...) and geoscience (atmosphere, continental drift ...). The driving mechanism of stripes in various systems is very different, but they follow common principles which are qualitatively explained as well as the driving mechanisms for selected examples. Besides stripes also hexagonal patterns (e. g. clouds, perma frost, vegetation patterns) squares, travelling or standing waves, oscillatory patterns, spirals (heart, chemical reactions etc.) or synchronization are explained. Most of the patterns are driven by dissipative (competing) processes and others by competing length scales. The formation of patterns is essentially a bifurcation. The generic types of bifurcation scenarios are discussed and analyzed by elementary textbook methods.

What is a stability band of spatial patterns? What is the number $\sqrt{3}$ in this context, for instance for Turing patterns? Is the Eckhaus-stability ratio $\sqrt{3}$ also relevant for an understanding of the dynamics of the skin-pattern of the "zebra"-fish as it is for instance in fluids? Is biological pattern formation purely driven by genes?

Optional: Using Matlab software for simulation and visualization of the dynamics of a few patterns.

Timeframe: 11.02. – 13.02 and 25.2-14.3 (1 full day)



B: Physical Properties of Liquid Crystals: From Low Molecular Weight Materials to Elastomers

Helmut Brand, Theoretical Physics III

The field of liquid crystals will be introduced. In one special topic we cover selected LC phases. The second special topic deals with physical properties and methods. In the project afternoon we will discuss selected literature and in particular the derivation of the Frank elastic energy for a nematic liquid crystal.

Time frame: 03.-07.03., 03./04.03., or 25.-28.03. (two times half a day)

B: Orbitals as a tool for understanding electronic structure

Stephan Kümmel, Theoretical Physics IV

The concept of orbitals is frequently used in molecular science to interpret experimental results and to develop an understanding of molecules. For example, in the context of light harvesting and solar cell research, the question of whether an excitation is characterized as having "charge transfer character" is typically discussed with the help of orbitals. However, from the perspective of physics an "orbital" is not a well defined object. There are different types of orbitals, and different orbitals typically carry different physical or chemical information. Therefore, "looking at orbitals" can either be helpful or it can be grossly misleading. In this topic the quantum mechanical concepts that are needed to understand and correctly interpret molecular orbitals will be explained. Organic molecular semiconductors will serve as examples.

Time frame: 21.03. or 07.04. (1 full day)

B: Diffusion in Polymers

Werner Köhler, Experimental Physics IV, Polymer Physics

Diffusion, the uncorrelated motion of molecules, plays a key role in understanding dynamic processes in macromolecular systems. In the first part of this topic basic concepts of how polymers diffuse in the bulk and in solution are introduced. The difference between self and collective diffusion is discussed and it is shown that a temperature gradient can also induce mass diffusion.

Relevant experimental techniques for the measurement of diffusion coefficients are discussed in the second part, and state of the art experiments can be seen in the laboratory.

The lectures will cover phenomenology of diffusion, including polymer models, linear laws, self diffusion, collective diffusion and thermal diffusion. As experimental techniques, light scattering and transient holography will be covered.

Time frame: 27.03. or 01.04. (1 full day)

B: Advanced Laser Techniques: Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscopy and Holographic Data Storage

Lothar Kador, BIMF

Confocal microscopy is a powerful technique for imaging samples in all three dimensions of space. It can easily be combined with the analysis of secondary radiation such as, *e.g.*, Raman scattering or fluorescence light. We will especially discuss the methods of confocal Raman microscopy, which yields information on the chemical composition of the sample, and confocal fluorescence lifetime imaging (FLIM) microscopy, which maps the excited-state lifetime of fluorophores. In the latter case, emphasis will be laid on experiments in the frequency domain which use a cw laser amplitude-modulated in the radio-frequency (rf) regime. In this context, some fundamentals of rf experiments will be touched. In the second part of the lecture, an introduction to holography and its application to high-density data storage in polymers will be given. The project part will be devoted to practical demonstrations of one of these techniques.

Time frame: 1 full day according to students' suggestions (except 30.03.-04.04.)

B: Kernmagnetische Resonanzspektroskopie und Polymerdynamik

Ernst Rößler, Experimentalphysik II

Seit einigen Jahren existiert ein kommerzielles Field-Cycling (FC) NMR-Spektrometer, das es erlaubt, die Frequenzabhängigkeit der Spin-Gitter-Relaxation (insbesondere ^1H) zu messen. Diese „NMR-Relaxometrie“ unterscheidet sich wesentlich von der konventionellen NMR. Im Gegensatz zu letzteren wird im Fall der FC-NMR das äußere Magnetfeld zwischen einem Polarisations-, Relaxations- und Detektionsfeld schnell (ms) geschaltet („Cycling“). Damit lassen sich u.a. Theorien der Polymerdynamik, wie z.B. das Doi-Edward'sche Tube-Reptation-Modell, erstmals über einen großen mikroskopischen Zeitbereich überprüfen. In Analogie zu rheologischen Messungen werden aus den Relaxationszeiten $T_1(\omega)$ Masterkurven konstruiert, die nach Fourier-Transformation es erlauben, die segmentale Korrelationsfunktionen über mehr als acht Dekaden in der Zeit zu verfolgen. Die Korrelationsfunktion weist unterschiedliche Potenzgesetzregime auf, die verschiedenen Arten der Polymerdynamik, wie Glas-, Rouse- und Entanglement-Dynamik, zugeordnet werden. Man kann hier von molekularer Rheologie sprechen. – Im experimentellen Teil werden Sie Messungen an einem solchen FC-NMR-Spektrometer durchführen, wobei die Kettenlänge (Molekulargewicht) des Polymers (Polybutadien) vom Grenzfall monomere Flüssigkeit bis hin zum Hochpolymeren variiert wird. Auf diese Weise wird der Übergang von einfacher Flüssigkeitsdynamik zur Polymerdynamik erkennbar und die besagten Relaxationsregime identifizierbar.

Time frame: to be announced (2 half days including experiments)

B: Biopolymer-based biofabrication for regenerative tissue engineering

Thomas Scheibel, Hendrik Bargel, Biomaterials

Modern regenerative medicine aims at the functional regeneration of tissue through stimulation and support of the endogenous regeneration potential of the human body. This approach longs for novel materials for bone, ligament and skin substitutes or nerve regeneration characterized by their defined three-dimensional structure, a tissue-related hierarchical morphology, and an adjusted biochemical composition. In order to gain such biomaterials, multidisciplinary approaches combining materials science and processing technologies, natural sciences and medicine are necessary. Biofabrication is an emerging field in the area of biomaterials, aiming at the generation of three-dimensional structures from materials that may contain vital cells and that allow the generation of scaffolds with high survival rates of the embedded cells. Suitable biopolymers such as silk proteins can be processed using different technologies, involving various spinning and coating methods as well as hydrogel formation. The resulting material morphologies have to be both mechanically and physically tested as well as analyzed concerning their cell compatibility and ability to promote suitable 2- and 3-D scaffolds for tissue engineering.

In this module, theoretical introductions into and demonstration of several processing methods of the model biopolymer spider silk protein including electro-spinning, dip-coating etc., biofabrication techniques, and biomedical characterization are given.

Time frame: 03.-06.03. or 07.-10.04. (2 afternoons 13:00 - 18:00)

B: Polymer foams

Volker Altstädt, Clemens Keilholz, Polymer Engineering

Due to the unique properties of polymer foams, a large number of innovative applications can be realized. These include packaging with reduced material costs, aerospace and automotive parts with good property-to-weight ratios, decreased thermal conductivity, and enhanced acoustic and mechanical damping.

The first part of the module focuses on the fundamental physics of polymer foams, including a detailed discussion of the foaming processes currently utilized both in academia and in industry as well as the resulting structure-property-relationships. Thereby, different types of polymer foams (particle foams, reactive polyurethane foams (PUR), extruded and injection-molded foams) and their typical properties and applications are introduced. In addition, current scientific approaches towards the control of cell nucleation, cell growth and volume expansion will be presented. Innovations (micro- to nano-cellular) and the hierarchical structuring of polymeric foams are also highlighted. Finally, the students will learn how to obtain tailored foam morphologies – and properties.

This oral part is followed by an experimental session taking place in our laboratories and pilot plant stations. More precisely, a practical introduction into foam injection-molding and foam extrusion is given using commercial machines. Finally, new trends and promising approaches as well as remaining questions will be discussed with the “foaming experts” of Polymer Engineering group.

Time frame: to be announced (1 full day)